F1G. 1

		· T		· ·		T		
CHOLESTEROL		→	->	→	+	→	1	
CARDIOVASCULAR		11	-	←				
UTERUS		←	*	→	→	←	*	—
BONE		—	+	←	->	←	-	-
BREAST		4		->	→			*
EFFECT	COMPOUND NAME	ESTRADIOL	TAMOXIFEN	RALOXIFENE	ICI 182, 870	NAFOXIDINE	CLOMIPHENE	PREMARIN

GST

HBD N-term

EP.

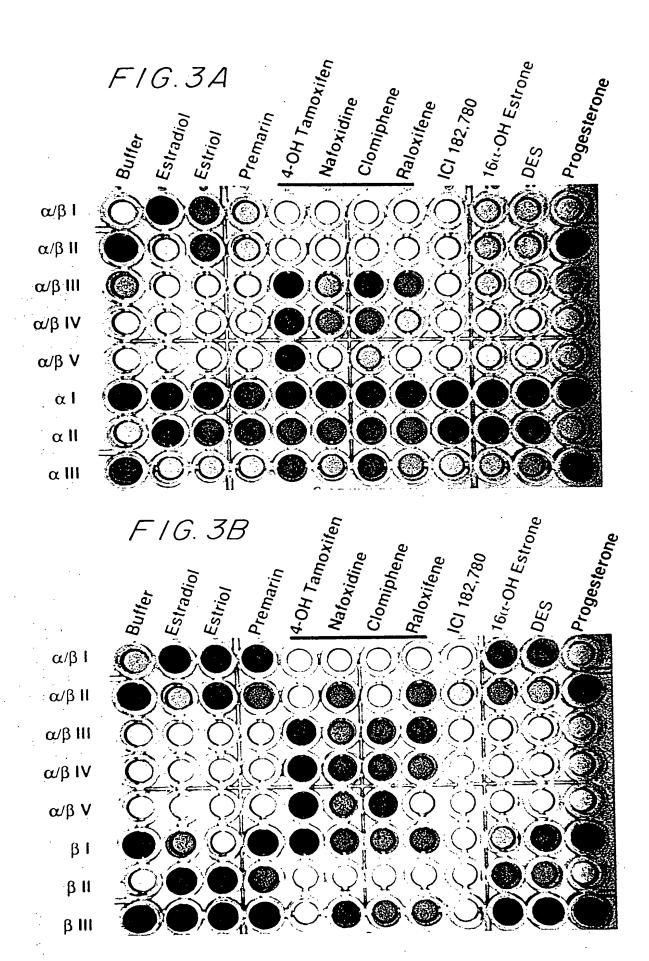
HBD N-term GST

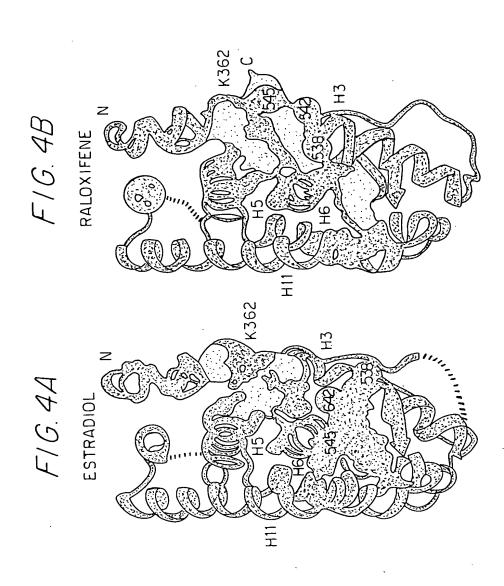
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F16.5A

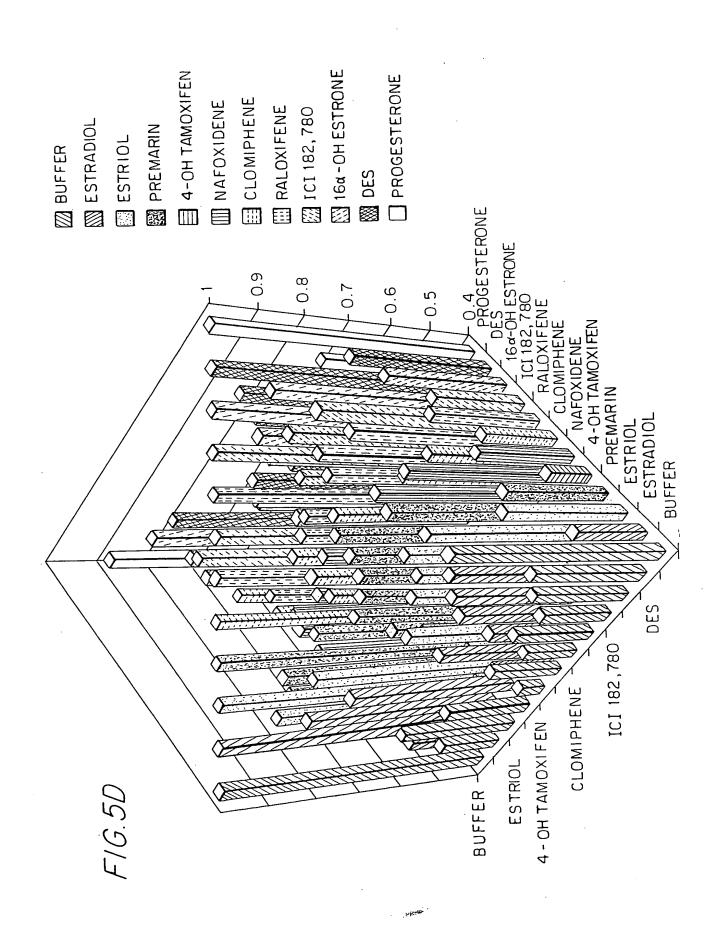
DES progesterone 2
raloxifene ICI 182,780 16α-OH estrone DES progesterone 1 1 2 2 1 4 1 2 2 1 2 2 1 2 0 1 1 1 1 1 1 1 1 1 6 6 6 6 5 4 1 2 2 3 4 4
raloxifene 1 1 4 7 7 2
clomiphene 1 1 6 7 7 5
nafoxidene 1 1 4 4 7 7 7
4-OH Tamoxifen nafoxidene clomiphene 1 1 1 1 1 6 4 4 4 6 6 7 7 7 7 7 7 7 7 5 6 6 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
premarin 2 2 1 1 6 6
estriol pi
estradiol e 6 2 1 1 1 1 1 2 2 6 6 6 6 6 6 6 6 6 6 6
buffer 7 7 1 1 1 7 7
αβ1 αβ11 αβ11 α Δ Ι Ι Ι Ι Ι α α Δ Ι Ι Ι Ι α

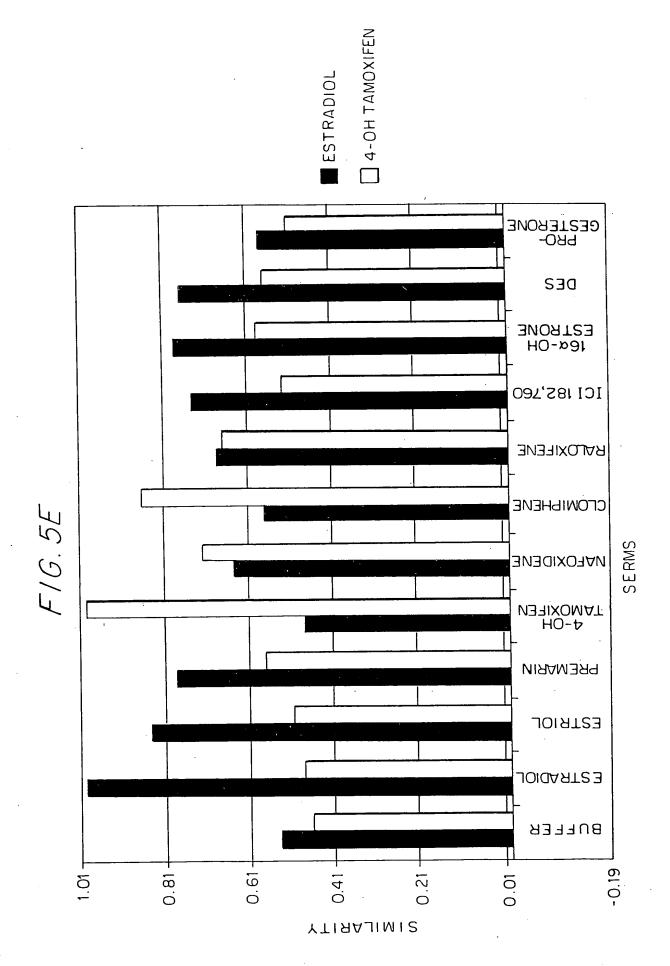
F16.5B

		•
19.8 9.79898987 15 16.03121954	2 8.485281374	6.782329983 9.797058971 7.211102551 8.306623863 6.708203932 7.549834435 6.08276253
19.8 15	6.32 4.69 3.32	2.45 6 8.6 9 7 4.69 7 6.56 8 4.12 6 1.73 1.73 0 5.29
19.79898987 15.26433752	7.280109889 4.358898944 3.16227766	1 2.45 8.306623863 8.6 4.123105626 4.69 6.164414003 6.56 3.464101615 4.12 2.449489743 3 0 1.73 6.08276253 5.29
19.79899 17.406895	8.4261498 5.1961524 4.472136	2.236068 9.4339811 5.3851648 7.2111026 4.2426407 0 2.4494897 3 7.5498344
19.79899 15.45962	8 6.324555 5.385165	3.464102 6.480741 2 4.358899 0 4.123106 3 3.741657 6.63325
19.79899 15.748016	9.3273791 8.4261498 7.8740079	6.244998 2.6457513 3.8729833 0 4.3588989 7.2111026 6.164414 6.5574385 8.3066239
19.79899 15.165751	8.4852814 6.9282032 6.0827625	4.472136 5.4772256 0 3.8729833 2.236068 5.3851648 4.1231056 4.6904158
19.79898987 17.40689519	10.67707825 10.19803903 9.746794345	8.366600265 0 5.477225575 2.645751311 6.480740698 9.433981132 8.306623863 8.602325267
19.799 · 15.6205	7.87401 4.24264 3.31662	0 8.3666 4.47214 6.245 3.31662 2.23607 1 2.44949 6.78233
19.8 15.46	6.557 3 0	3.317 9.747 6.083 7.874 4.899 4.472 3.162 3.317 5.916
19.799 16.7033	9.16515 0 3	4.24264 10.198 6.9282 8.42615 6.32456 5.19615 4.3589 4.69042 8.48528
19:799 17.407	0 9.1652 6.5574	7.87 10.677 8.4853 9.3274 8.4261 7.2801 6.3246
Universal Max Max	buffer estradiol estriol	5.916079783 premarin 4-OH Tamoxifen 10.677 nafoxidene 8.4853 clomiphene 9.3274 raloxifene 9.3274 raloxifene 1C1 182.780 16α-OH estrone 7.2801 DES 6.3246 progesterone 2

F16.5C

progesterone 0.898985 0.571429 0.701193 0.657441 0.505128 0.635784 0.580452 0.661185 0.61185 0.618676 0.692774 0.732739
DES 0.680562 0.763098 0.832485 0.876282 0.565517 0.763098 0.668799 0.791752 0.848477 0.912518
16α-OH es 0.632299 0.779842 0.840281 0.949492 0.580452 0.791752 0.68865 0.825036 0.876282 1 0.912518 0.692774
CI 182,780 0.574415 0.737555 0.774123 0.887062 0.523512 0.728008 0.635784 0.785714 1 0.876282 0.848477
raloxifene 0.595939 0.680562 0.728008 0.825036 0.672673 0.898985 0.779842 0.779842 0.848477 0.811018 0.66497
clomiphene 0.528896 0.574415 0.602303 0.68458 0.866369 0.804385 0.779842 0.635784 0.68865 0.668799
nafoxidene c 0.571429 0.650073 0.692774 0.774123 0.723358 0.804385 0.887062 0.728008 0.791752
4-OH Tam ni 0.460726 0.484921 0.507713 0.577423 0.577423 0.573358 0.866369 0.672673 0.523512 0.523512 0.523512
premarin 0.602303 0.785714 0.832485 0.577423 0.774123 0.68458 0.832485 0.832485 0.832485 0.832485
Φ
buffer estradiol estradiol estradiol 0.53709 1 0.53709 1 0.53709 1 0.568799 0.848477 0.602303 0.785714 0.0602303 0.785714 0.0771429 0.650073 0.528996 0.574415 0.528996 0.574415 0.528996 0.574415 0.52899 0.779842 0.680562 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.763098 0.680562 0.774429
buffer estradiol cstradiol opremarin 4-OH Tamoxifen 0 nafoxidene clomiphene raloxifene 0 16α-OH estrone 0 DES





F16.64

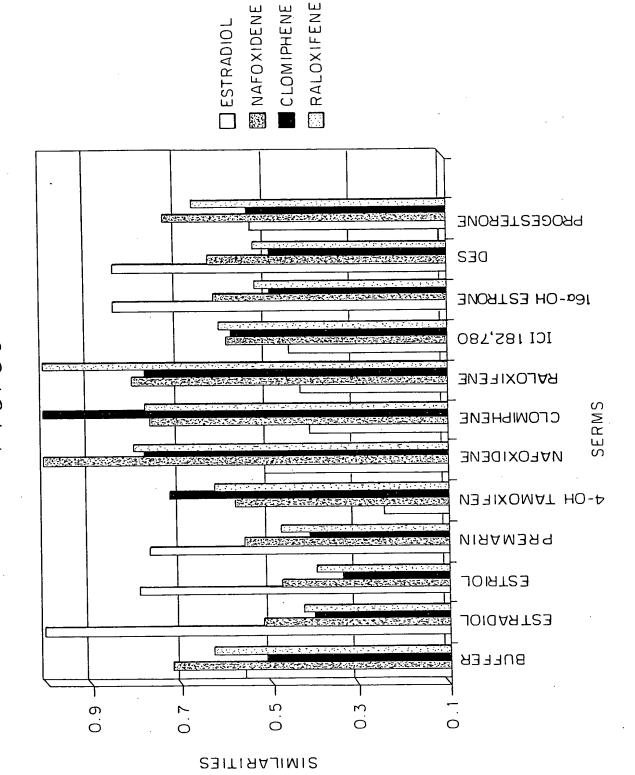
a	_	9	-	-	-	2	0	2
4-OH Tamoxifen nafoxidene clomiphene raloxifene ICI 182,780 16α-OH estrone DES progesterone	2	က	-	-	-	4	· co	7
)H estrone	2	က	-	-	-	2	က	7
CI 182,780 16α-(0	7	-	-	0	0	0	-
raloxifene	0	4	9	4	2	4	0	က
clomiphene	0	-	2	5	2	က	0	က
nafoxidene	-	4	က	2	က	4	0	2
4-OH Tamoxifen	0	-	7	7	7	7	0	•-
	9	4	•	-	-	7	4	
estriol	7	9		-	-	8		
ouffer estradiol estriol premarin	7	2	-	-	-	က	ص	7
buffer	2	7	2	2	-	9	-	7
	αβ I	αβ 11	αβ !!!	β.I) II s	β III	ΙΛΩ	βV

F16.6B

Universal Max Max	16.76305	16.79899 16.76305 16.49242 17.4069		16.55295	16.55295 19.13112647	14.106736	15.524175	14.93318	18.1383571	14.106736 15.524175 14.93318 18.1383571 15.45962483 15.16575 16.70329309	15.16575	16.70329309
buffer estradiol	0 8.774964	8.774964 8	9.306624	0 8.774964 8.306624 6.082763 54 0 4.242641 4.690416	12.80624847 15.32970972	5.7445626	10 11.789826	7.416198	10 7.416198 10.2469508 789826 11.40175 10.9544512	6.8556546 3.16227766	5.91608	5.91608 3.16227766 3.162278 9.219544457
estriol	8.306624	3.306624 4.242641	0	5.830952 1 6		10.392305	13.228757	12	-	4.69041576	5.09902	5.09902 9.219544457
premarin 6.082763 4.690416 5.830952 0	6.082763	5.082763 4.690416 5.830952 12 80626 15 22071 16 70220	5.830952	0	14.31782106	8.8317609 8.4261498	11.874342 5 6568542	10.58301	11.9163/53	5.291502622		3.464102 7.280109889 13 82027 12 40967365
nafoxidene	5.744563	9.69536	5.744563 9.69536 10.3923	8.831761	8.45	0.41024.0	4.7958315	4.00510.1	8.1240384	7.615773106	7.348469	7.348469 5.385164807
clomiphene	9	10 11.78983 13.22876	13.22876	11.87434		4.7958315	0	4.582576	4.582576 8.42614977		10.14889	9.055385138
raloxifene	7.416198	11.40175		8.774964	7.615773106	4	4.5825757	0	7.87400787	9.486832981 9.273618 6.708203932	9.273618	6.708203932
ICI 182,780	10.24695	10.95445	10.24695 10.95445 11.91638	11.91638	13.07669683	8.1240384	8.4261498	7.874008	0	8.717797887 9.380832 7.681145748	9.380832	7.681145748
16α-OH estrone	6.855655	3.162278	6.855655 3.162278 4.690416		14.38749457	7.6157731	10.148892	9.486833	9.486833 8.71779789	0	2	6.8556546
DES	5.91608	5.91608 3.162278 5.09902	5.09902	.,	13.82027496 7.3484692	7.3484692	10.148892	9.273618	9.273618 9.38083152	2		0 6.244997998
progesterone	3.162278	3.162278 9.219544 9.219544	9.219544	7.28011	12.40967365 5.3851648	5.3851648	9.0553851	6.708204	6.708204 7.68114575	6.8556546 6.244998	6.244998	0

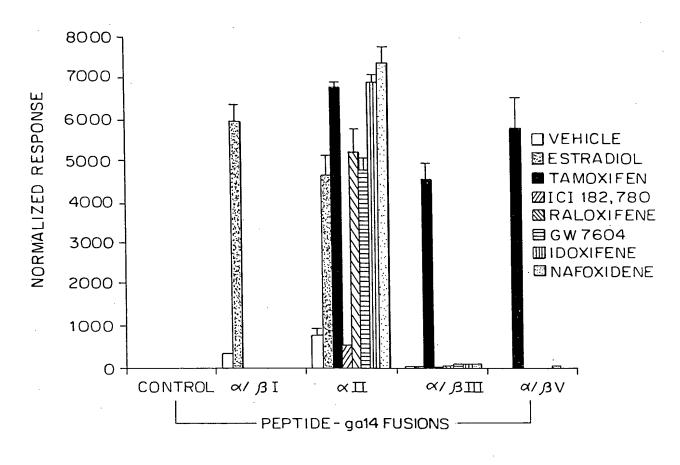
F16.6B

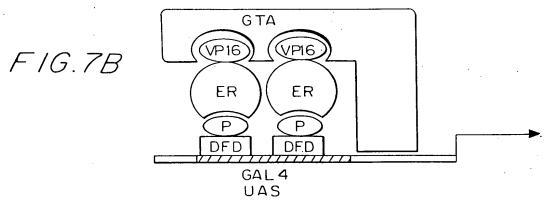
	9	, ici	loi 100		A.OH Tam	anatovidana	clominhene	raloxifone	ICI 182 780	16α-OH es	DES	progesterone
huffer	onlier +	25(140)01 0 556797	0.58042	. 0 692774098	0.353187	0.709856	0.494924	0.625425	0.482451	0.653737	0.701193	0.840281
estradiol	0.556797		0.785714		0,225733	0.51031	0.404524	0.424124	0.446717	0.840281	0.840281	0.534343
estriol	0.580452	0.785714			0.156356	0.475109	0.331847	0.393908	0.398132	0.763098	0.742461	0.534343
nremarin	0.692774	763098	0.705492		0.276841	0.553929	0.400255	0.465478	0.398132	0.732739	0.825036	0.632299
4-OH Tamovifen	0.353187	0.225733		0.276840831	•	0.574415	0.714286	0.618676	0.339527	0.273322	0.301971	0.373217
nafoxidene	0.709856	0.51031		0.553928714	0.574415	-	0.757774	0.797969	0.589674	0.615345	0.628846	0.728008
clominhene	0.494924	0 404524		0.400255156	0.714286	0.757774	,	0.768545	0.574415	0.487404	0.487404	0.542634
raloxifene	0.625425	0 424124		0.55679737	0.615345	0.797969	0.768545	-	0.602303	0.520843	0.531612	0.661185
ICI 182 780 0 482451 0	0.482451	0.446717		0.398132159	0.339527	0.589674	0.574415	0.602303	-	0.559685	0.526196	0.612044
16v-OH estrone	0.653737	0.840281		0.732738758	0.273322	0.615345	0.487404	0.520843	0.559685	-	0.898985	0.653737
DES	0.701193	0.840281		0.825036447	0.301971	0.628846	0.487404	0.531612	0.526196	0.898985	-	0.68458
sterone	0.840281	0.534343	0.534343	0.632298924	0.373217	0.728008	0.542634	0.661185	0.612044	0.653737	0.68458	-

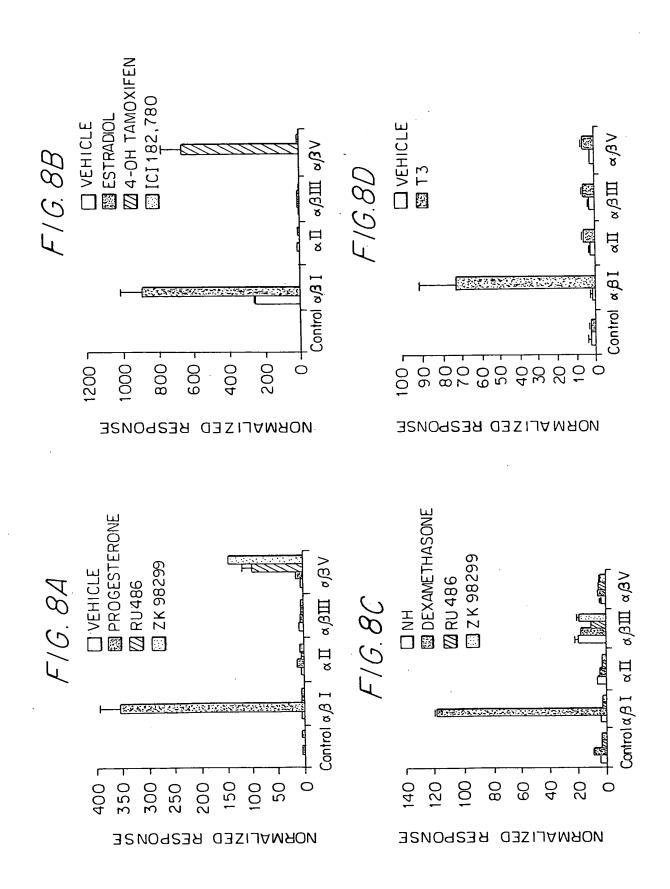


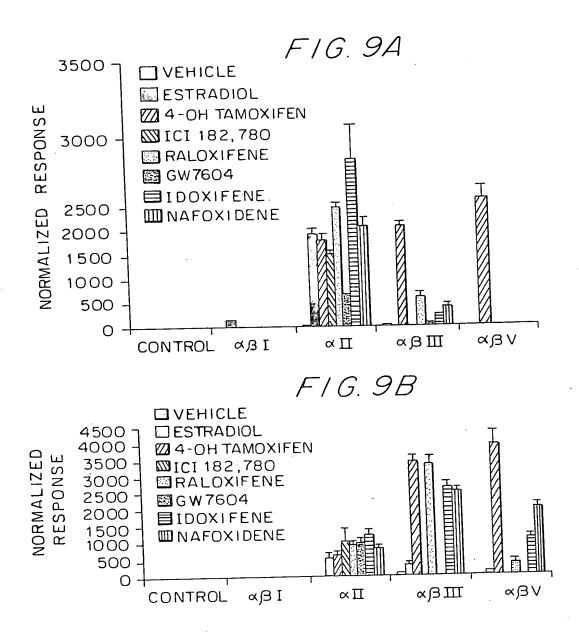
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FIG. 7A

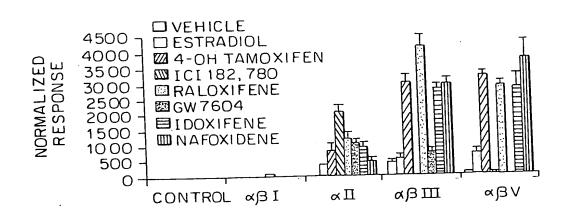


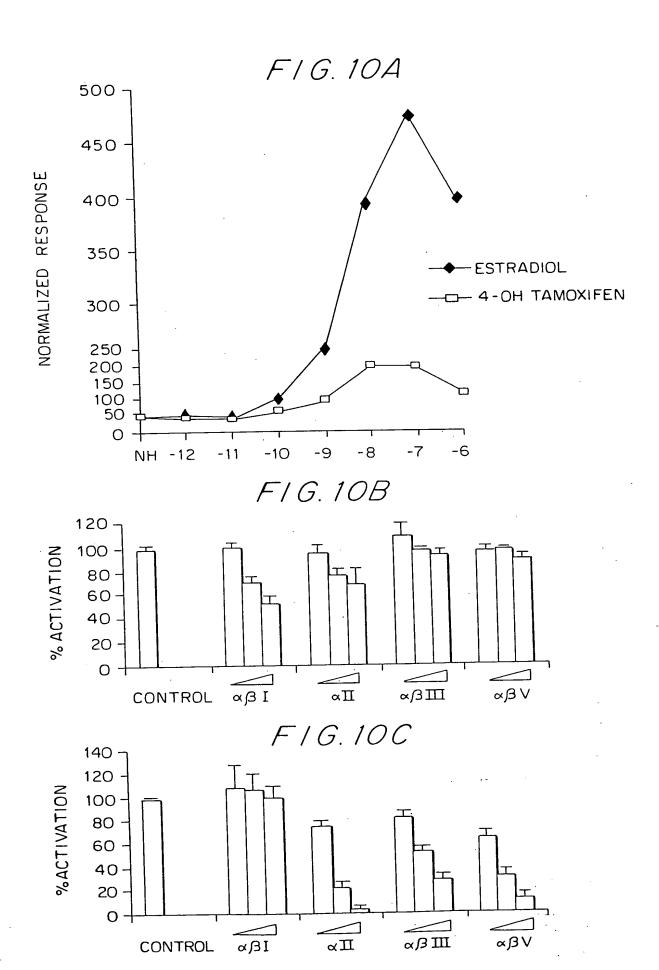


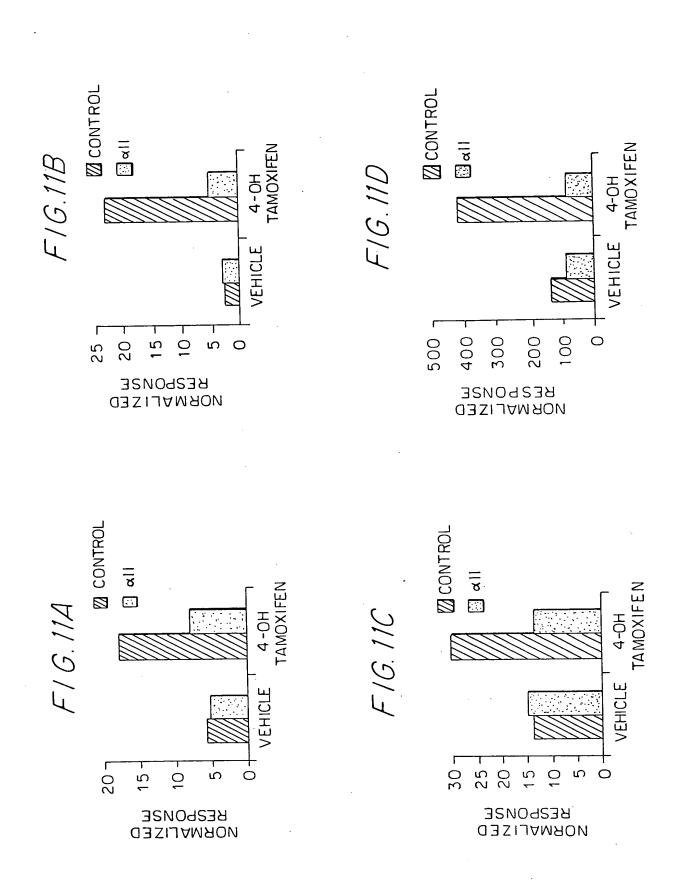




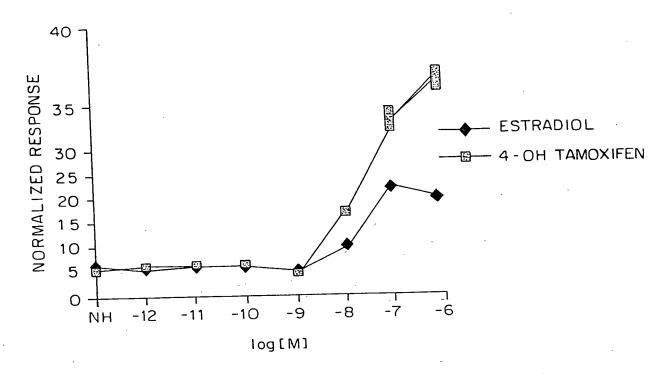
F1G.9C



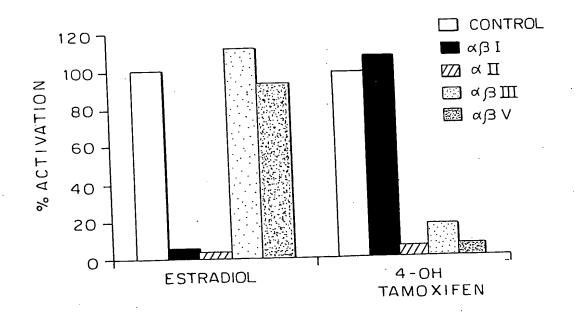


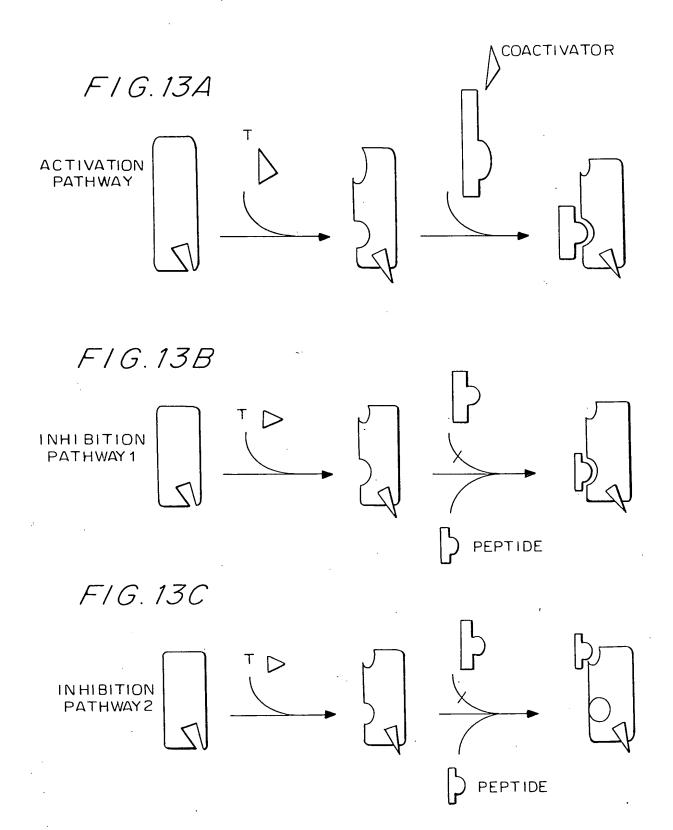


F1G. 12A



F1G.12B





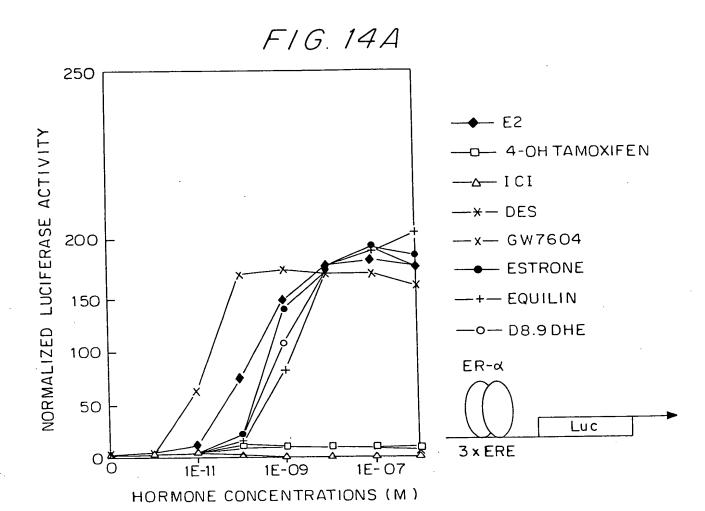
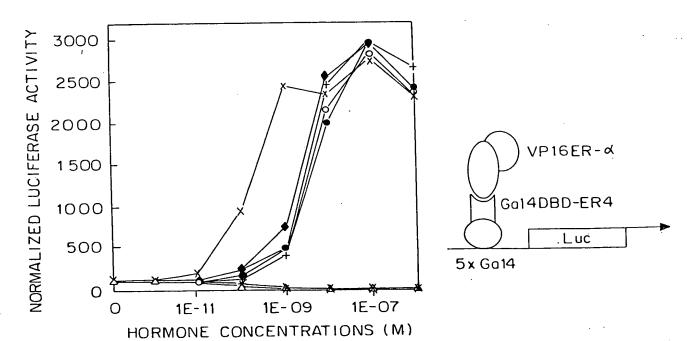
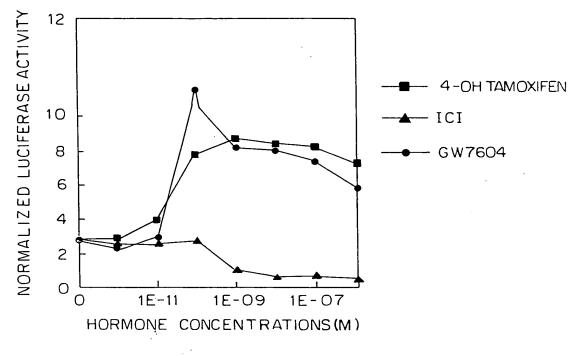


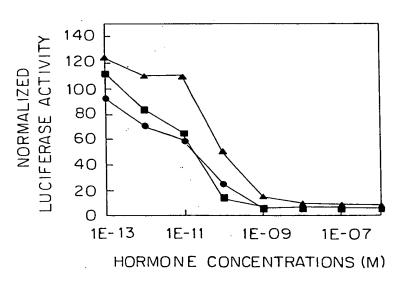
FIG. 14B

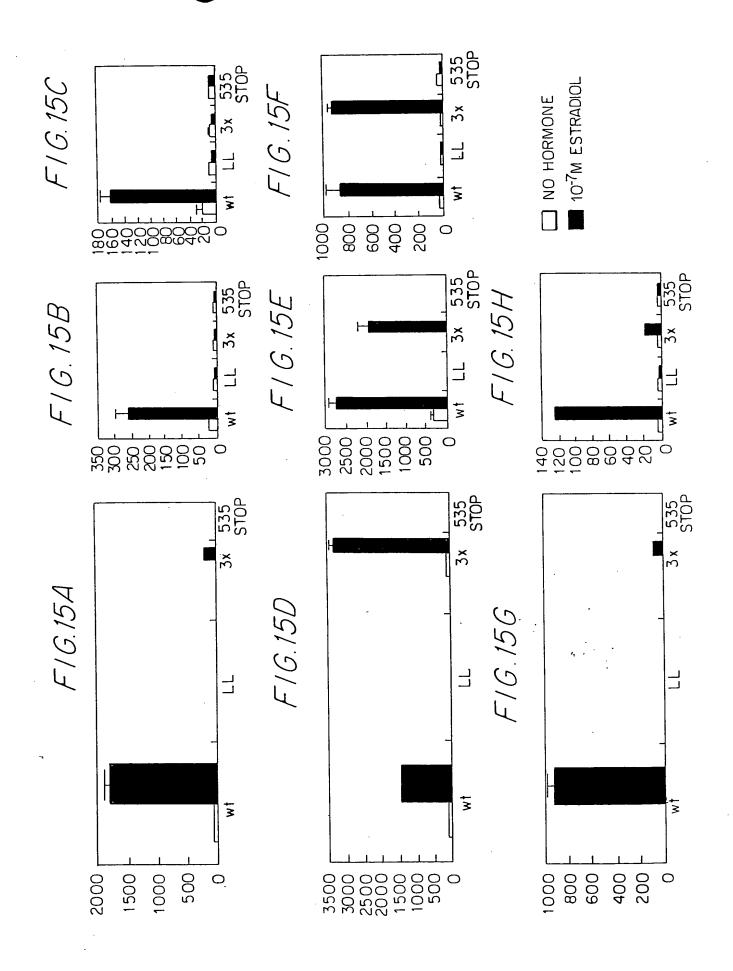


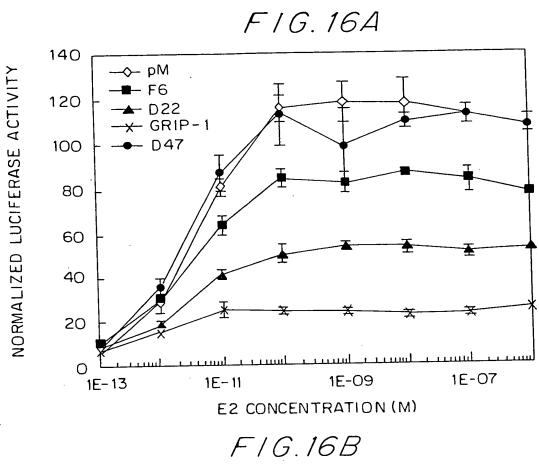
F1G. 14C

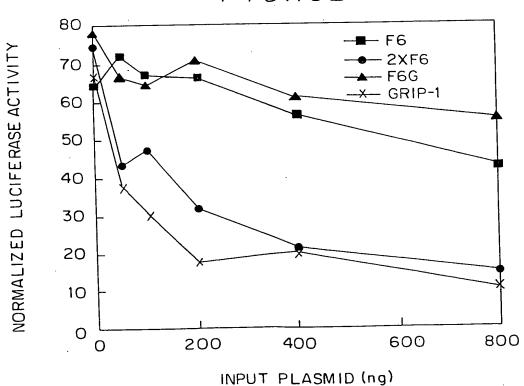


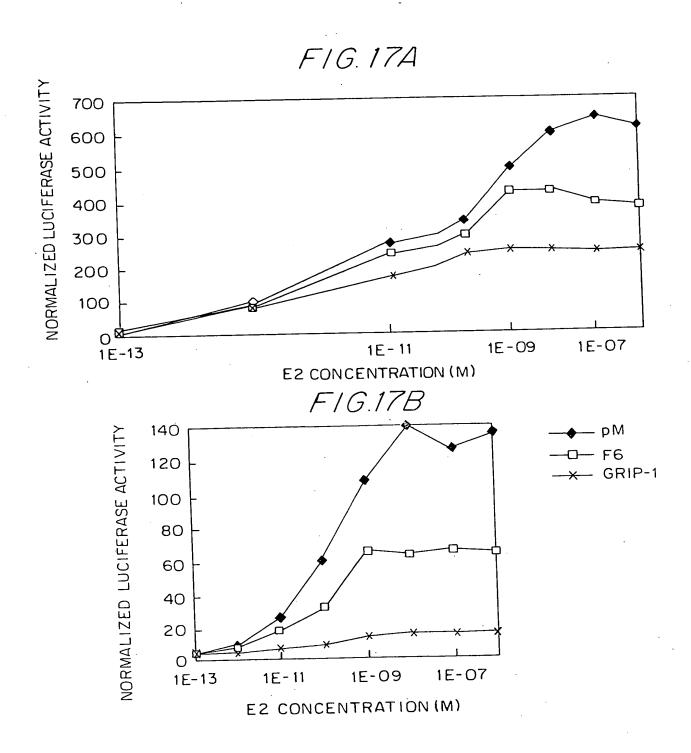
F1G. 14D











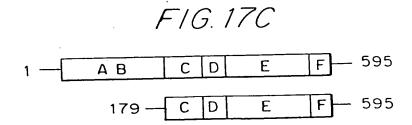
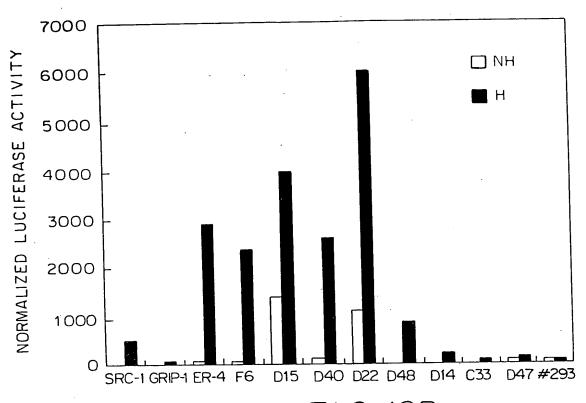


FIG. 18A



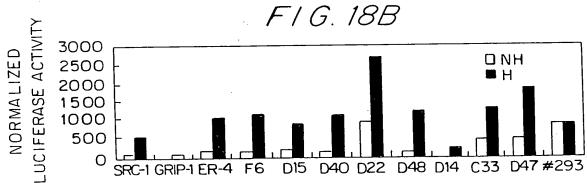
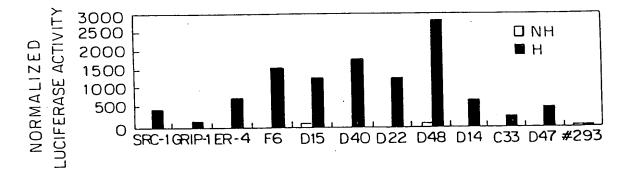
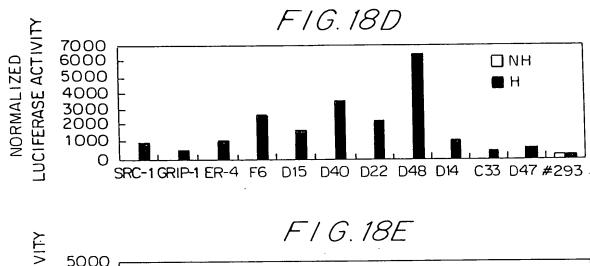
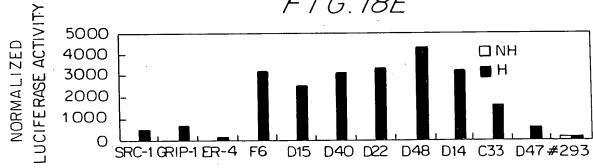


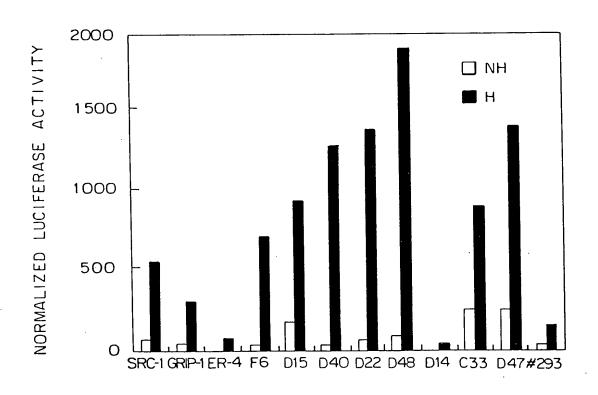
FIG. 18C

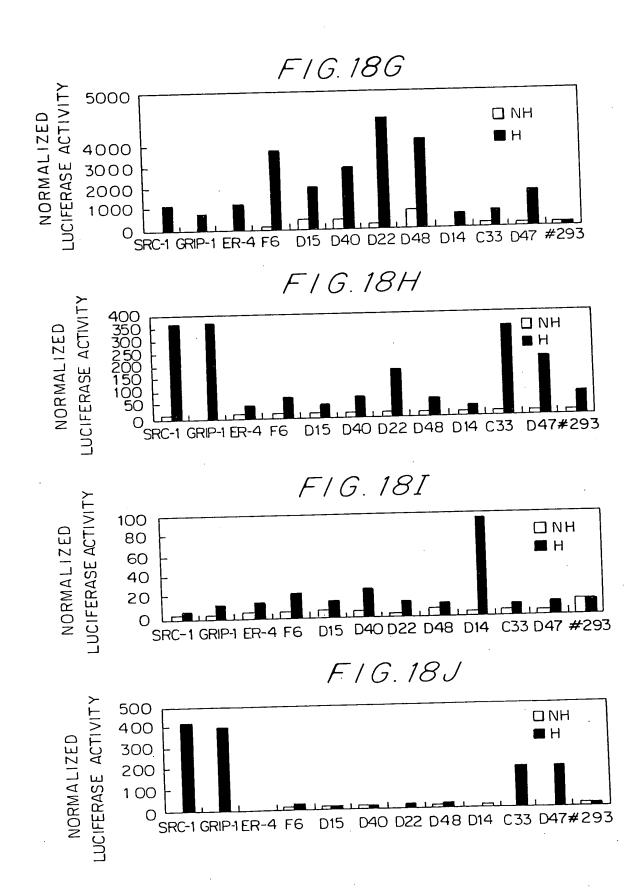


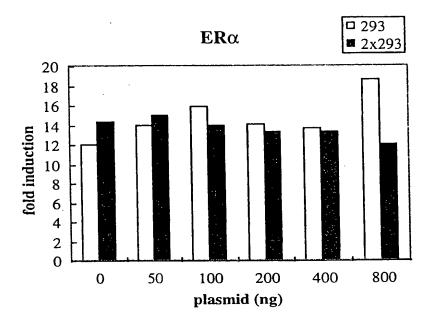


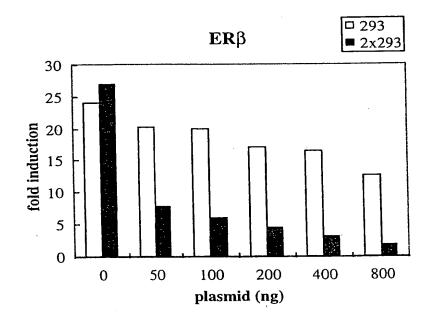


F1G.18F







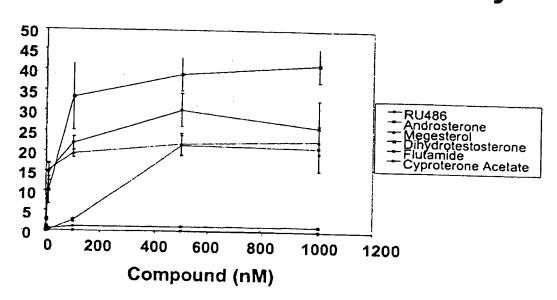


F/G. 78

Nafox 2.053 3.324 7397 63.84 8.434	6651.107 6556.022 7467.322 6889.769 2152.019 2592.036 472.2028 0	0.60 0.55 0.58 0.87 0.97 1.00
ldox 2.294 4.256 6925 60.2	6179.562 6372.767 7437.648 6417.774 1680.089 2120.054 0 472.2028	0.61 0.55 0.61 0.90 0.87 1.00 0.97
7604 1.414 16.08 4805 64.21 13.2	4062.318 5947.69 7709.347 4297.842 440.2544 0 2120.054 2592.036	0.73 0.53 0.74 0.97 1.00 0.87
Ralox 2.031 6.449 5245 56.18 5.059	4501.922 5983.961 7617.299 4737.759 0 440.2544 1680.089 2152.019	0.73 0.64 0.54 0.71 1.00 0.97 0.90
1CI 0.845 1.359 507.3 33.15 7.16	381.3001 7266.298 9777.12 0 4737.759 4297.842 6417.774 6889.769	0.98 0.56 0.41 1.00 0.71 0.61
3.076 8.54 6821 4696 5837	9627.63 9787.266 0 9777.12 7617.299 7709.374 7437.648	0.42 0.41 1.00 0.54 0.53 0.55
E2 1.621 5962 4663 34.67 9.313	6886.618 0 9787.266 7266.298 5983.961 5947.69 6372.767	0.58 1.00 0.41 0.56 0.64 0.64
NH 1.341 293.5 752.3 32.93 2.901	0 6886.618 9627.63 381.3001 4501.922 4062.318 6179.562 6651.107	1.00 0.58 0.42 0.98 0.73 0.75 0.63
control AB1 A2 AB3 AB5	NH dist E2 dist OT dist ICI dist Ralox dist 7604 dist Idox dist Nafox dist	NH sim E2 sim OT sim ICI sim Ralox sim 7604 sim Idox sim

<u>AR</u>

Conformational Response Assay



Lady Marie Control and the the Control of the Control of the Control of Contr